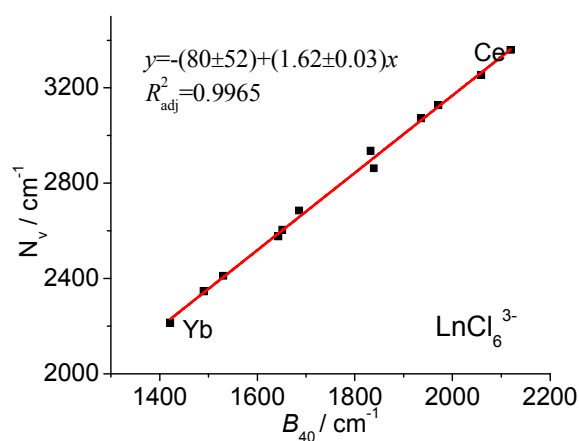


# Electronegativity, charge transfer, crystal field strength and the point charge model revisited

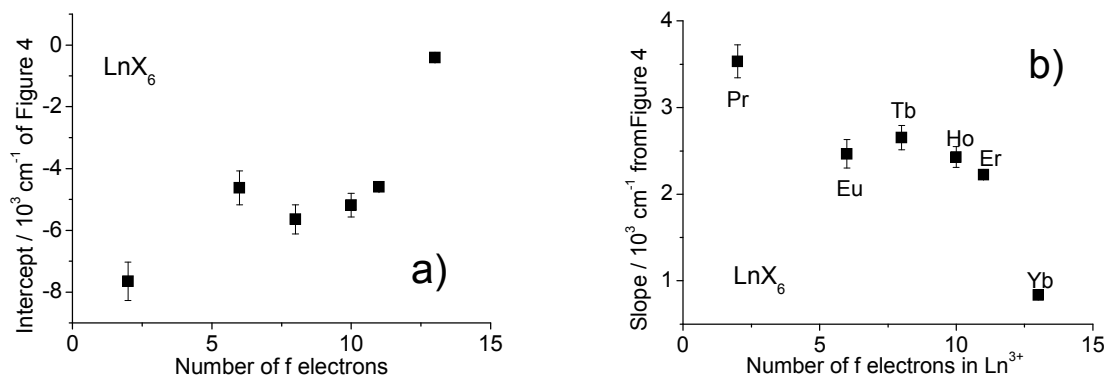
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**Figure S1.** Plot of  $N_v$  against fourth rank crystal field parameter for  $\text{LnCl}_6^{3-}$  systems.



**Figure S2.** Plots of a) intercept and b) slope from Figure 4 (i.e. linearity of  $N_v$  and electronegativity for  $\text{LnX}_6$  moieties).

Table S1. Radial integrals and crystal field parameters for tripositive lanthanide ions in Cs<sub>2</sub>NaLnCl<sub>6</sub> systems from Duan, C. -K.; Tanner, P. A. *J. Phys. Chem. A* **2010**, *114*, 6055-6062.

| Ln <sup>3+</sup>                                          | Ce     | Pr    | Nd    | Pm     | Sm    | Eu    | Gd    | Tb    | Dy    | Ho    | Er    | Tm    | Yb    |
|-----------------------------------------------------------|--------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| <i>N</i>                                                  | 1      | 2     | 3     | 4      | 5     | 6     | 7     | 8     | 9     | 10    | 11    | 12    | 13    |
| $\langle r^2 \rangle$ (10 <sup>-20</sup> m <sup>2</sup> ) | 0.373  | 0.347 | 0.322 | 0.300  | 0.281 | 0.265 | 0.250 | 0.237 | 0.226 | 0.215 | 0.206 | 0.197 | 0.189 |
| $\langle r^4 \rangle$ (10 <sup>-40</sup> m <sup>4</sup> ) | 0.316  | 0.279 | 0.241 | 0.211  | 0.187 | 0.168 | 0.151 | 0.138 | 0.126 | 0.115 | 0.106 | 0.099 | 0.092 |
| $\langle r^6 \rangle$ (10 <sup>-60</sup> m <sup>6</sup> ) | 0.507  | 0.430 | 0.350 | 0.292  | 0.247 | 0.212 | 0.185 | 0.162 | 0.144 | 0.128 | 0.115 | 0.104 | 0.095 |
| <i>B</i> <sub>40</sub> (cm <sup>-1</sup> )                | 2119.5 | 2059  | 1971  | [1958] | 1832  | 1936  | 1839  | 1686  | 1652  | 1643  | 1531  | 1491  | 1422  |
| <i>B</i> <sub>60</sub> (cm <sup>-1</sup> )                | 260.7  | 237   | 249   | [24]   | 274   | 245   | 112   | 228   | 178   | 151   | 160   | 152   | 86    |